PROJECT - PART A

① INITIAL CONFIGURATION :

$$N = 108$$

$$L_x = L_y = L_z = 18.0 \text{ Å}$$

$$\epsilon = 0.238 \text{ KCAL/MOL}$$

$$\sigma = 3.4 \text{ Å}$$

GENERATE A RANDOM INITIAL CONFIGURATION

$$(r_{ij} \geq 3.4 \text{ Å})$$

② $$U_{LJ}(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$$

↓ INTERACTION ENERGY PER PAIR

③ MINIMIZE THE TOTAL POTENTIAL ENERGY OF THE SYSTEM $-\nabla U| = 0$ (USE PERIODIC BOUNDARY CONDITIONS) min

④ CALCULATE THE HESSIAN MATRIX AND GET THE EIGEN VALUES AND EIGEN VECTORS.

⑤ GET THE HISTOGRAM OF VIBRATIONAL FREQUENCIES